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Work on the oxidation of the aromatics present in jet propulsion fuels has continued with the major effect now directed at the dialkylated benzenes. The major study concerned the oxidation of para-xylene. The results indicate the oxidation of one side chain at a time before the benzene ring is attached. There is a linear decay of the fuel and the major species detected were toluene, benzene, p-toluadehyde, p-ethyltoluene and CO. Kinetic steps leading to these intermediates are given. (continued on reverse)

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SUMMARY

After great progress related to soot formation in normal diffusion flames, studies of near and slightly sooting inverse diffusion flames were initiated to determine the key intermediates to soot formation. The results indirectly confirm that the initial number density of soot particles which form scale with aromatic formation just prior to soot inception. Correlations exist between a fuel's sooting tendency as measured by the Princeton smoke height experiment and the extent of aromatic formation measured in both inverse and normal diffusion flames.

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Combustion property observations of isolated boron slurry droplets were extended in the past year to in-house boron/JP-10 slurries with and without surfactants. The experimental results have revealed that stabilizing agents are responsible for the violent disruption of the primary slurry droplet and strongly support the hypothesis of the formation of the impermeable shell and subsequent disruption phenomena, that had been proposed previously.

I. Research Objectives

Present and anticipated variations in fuels and trends toward high performance propellants require greater understanding of the chemical

phenomena associated with the combustion aspects of the varicus propulsion systems of current and future interest to the Air Force. Under AFOSR an integrated, fundamental program on fuel research was established at Princeton. Current emphasis and research objectives are directed towards understanding soot formation and destruction processes; on related pyrolysis and oxidation studies of hydrocarbons, particularly the various types of aromatics that aggravate soot conditions and are the components of heavy fuels, and mastering high energy density boron and slurry combustion problems.

In subsequent sections this report details the progress made during the past year and the publications which have emanated from the work.

II. Status of the Research and Year's Progress

This section is divided into three parts which correspond to the current major objectives of the research program.

A. Pyrolysis and Oxidation of Aromatic Fuels

Previous investigations (1-3) of the high temperature (1000-1200K) oxidation of methyl, ethyl and n-propyl benzene in the Princeton flow reactor have indicated that three primary processes are instrumental in removing the alkyl side chain from the aromatic ring: 1) abstraction of a hydrogen from the alkyl group, decomposition of the radical and, oxidation of the subsequently formed species; 2) displacement of the alkyl group by a radical species-usually an H atom; 3) thermal cleavage (homolysis) of part of the side chain followed by oxidation of the resultant radicals. Since the side chain is removed initially by these three processes without any major attack on the aromatic ring (4,5), it was also found that the oxidation of alkylated aromatics eventually reduces simply to the oxidation of the phenyl radical and/or benzene. Much of the basic understanding of the reactions important in the

removal of the side chain was gained from observing that the chemistry of the oxidation of methyl, ethyl and n-propyl benzene was analogous in many ways to the oxidation chemistry of methane (6), ethane (7) and propane (8). Further experimental work in relation to earlier work on the oxidation of butane (9) showed that similar analogies could be made with n-butyl benzene (10). The consequence of this extensive work on the mono-alkylated aromatics was the formulation of a simple, generalized, mechanistic model for the oxidation of the monoalkylated aromatics that certainly should be valid in the temperature and pressure range of the turbulent flow reactor (10).

The main effort on this aspect of the overall program then concentrated on the multi-substituted aromatics with particular attention given to para-xylene. Most of the oxidation experiments on p-xylene were conducted in the range of 1163-1183K at a mixture ratio that was essentially stoichiometric. Data taken indicated that the stoichiometry did not affect the oxidation mechanism noticeably.

The major species detected during the experiments were toluene, benzene, p-tolualdehyde, p-ethyltoluene, CO, and fuel (Fig. 1). The major aliphatic found was methane. The concentration of CO increased throughout the oxidation process, hence, no CO_2 was formed and the experiments were essentially isothermal.

The fuel appears to decay linearly suggesting a zero order decomposition. This result is believed to be caused by the p-methylbenzyl radical $(CH_3C_6H_4CH_2)$. The intermediates formed during the oxidation indicate that this radical could be present in large amounts due to resonant stability. Consider the formation of ethyltoluene. The most likely means to form ethyltoluene is by the reaction between methylbenzyl and a methyl radical (the

methyl coming from a side chain displacement by hydrogen). For the radical-
radical reaction to be significant, relatively large amounts of methylbenzyl
and methyl must be present. The stability of methyl is well known. It is
postulated that methylbenzyl is resonantly stabilized, similar to the benzyl
radical ($C_6H_5CH_2$), hence allowing it to form in relatively large concentra-
tions. Further support would be the presence of larger aromatics such as 1,2-
di-(4-tolyl) ethane which can be formed by the dimerization of two methyl-
benzyl radicals. The positive identification of this species is currently
being investigated through the use of mass spectrometry.

In order to possibly explain the linear fuel decay one notes that the
sampling probe now in use quenches the sample at 70C so that unstable species
quickly recombine to form stable species. Thus if methylbenzyl were sampled,
it would most likely recombine with any hydrogen or abstract hydrogen from
other species and be detected as xylene. This effect could explain the
apparent linear rate of fuel decay seen in the data. Of course this
hypothesis must be verified through estimation of the methylbenzyl radical
concentration which is currently being done. It is worth pointing out that
previous oxidation experiments of toluene ($C_6H_5CH_3$) in the reactor also
produced a linear fuel decay and the benzyl radical was estimated to achieve
relatively high concentrations.

The proposed oxidation mechanism of p-xylene involves the oxidation of
one side chain at a time before the ring is broken in a manner not unlike the
oxidation of the single side chain species, toluene. The major reaction route
is the abstraction of the side chain hydrogen by a radical (X)

$$CH_3C_6H_4CH_3 + X \longrightarrow CH_3C_6H_4CH_2 + XH \tag{1}$$

Reaction (1) has been observed by other investigators to dominate over

addition of X at the temperature of this study. Trace amounts of dimethylphenol were detected though, probably due to the addition of O atom to the ring. Competing with (1), but less likely, is the displacement of the methyl group by hydrogen

$$CH_3C_6H_4CH_3 + H \longrightarrow C_6H_5CH_3 + CH_3 \qquad (2)$$

which has also been documented. This postulate is supported by the early appearance of large amounts of toluene and the presence of ethyltoluene as discussed earlier.

The methylbenzyl then reacts with O atom to form tolualdehyde, another major intermediate,
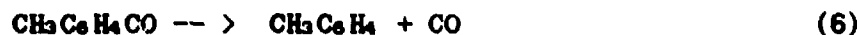
$$CH_3C_6H_4CH_2 + O \longrightarrow CH_3C_6H_4CHO + H \qquad (3)$$

or ethyltoluene

$$CH_3C_6H_4CH_2 + CH_3 \longrightarrow CH_3C_6H_4C_2H_5 \qquad (4)$$

The methylbenzyl can also dimerize, as noted earlier, but this step is not a significant reaction route.

The fate of the tolualdehyde is most likely abstraction of the formyl H and the decomposition to CO and the tolyl radical

$$CH_3C_6H_4CHO + X \longrightarrow CH_3C_6H_4CO + XH \qquad (5)$$

$$CH_3C_6H_4CO \longrightarrow CH_3C_6H_4 + CO \qquad (6)$$

This route is supported by the presence of early CO continuing throughout the oxidation from the beginning. The tolyl radical probably abstracts an H (e.g. from the fuel) and oxidizes as toluene since no aromatic ring fragments which contain the extra methyl group are detected.

Small amounts of p-methylstryrene were detected and are believed to come from the decomposition of the ethyltoluene via the abstraction of the benzylic hydrogen

$$CH_3C_6H_4C_2H_5 + X \longrightarrow CH_3C_6H_4CHCH_3 + XH \qquad (7)$$

$$CH_3C_6H_4CHCH_3 \longrightarrow CH_3C_6H_4CH=CH_2 + H \qquad (8)$$

Similar to reaction (2), the ethyltoluene can also have the ethyl group displaced by a hydrogen. The fate of the methylstyrene is probably displacement of the ethenyl group again leading to the tolyl radical.

The side chain of the toluene formed then oxidizes in a similar manner as the xylene until the phenyl radical (C_6H_5) is formed. This radical oxidizes to cyclopentadiene which breaks down into the aliphatics.

So, as can be seen by the suggested mechanism, it is believed that p-xylene oxidizes one side chain at a time and leads to formation of CO before the aromatic ring breaks up and the subsequent formation of toluene. The trend the mechanism suggests is supported by the experimental data obtained.

The current work will be directed towards determination of the concentration of the methylbenzyl radical to explain the linear fuel decay and to further develop the analysis techniques using capillary column gas chromatography. It is believed that improved analysis will yield more information on the trace species and their role in the oxidation. Finally, preliminary work has begun on the oxidation of the ortho- and meta- isomers and will continue to be investigated. Of particular interest is what change, if any, occurs in the o-xylene mechanism which leads to a faster burning time. Upon completion of the study of the xylenes, more detailed attention will be given to the polynuclear aromatics which form a component of JP fuels and have serious ramifications with respect to soot formation as well as environmental considerations. Because of earlier preliminary studies (11), the first compound to be studied will be 1-methylnaphthalene.

B. Soot Formation and Destruction Process

Extensive progress and understanding of soot processes have developed from this aspect of the AFOSR program. These Princeton studies were the first to clearly distinguish the difference between sooting tendencies of pre-mixed and diffusion controlled combustion processes and to emphasize the importance of considering temperature in analyzing the sooting tendency of fuels (12). The work on pre-mixed flames was completed and a correlation developed between the critical sooting equivalence ratio of fuels and mixtures and a single property of the fuel, namely the "number of C-C bonds" (13). Work on diffusion flames also has largely been completed. The importance of temperature was particularly significant for this type of combustion process. The results of the program make it possible to determine from a fundamental knowledge of the pyrolysis kinetics of component fuels, their tendency to soot under diffusion flame conditions (14,15).

The key to controlling soot formation irrespective of controlling the temperature is a knowledge of the mechanism of soot formation, but, perhaps, as important, also knowledge of the precursors that control the soot formation process. Thus for this annual period most attention was directed towards this objective by chemical sampling "unique" inverse diffusion flames and making use of the chemical instrumentation available in the oxidation kinetics aspect of the program. The sampling for these flames is performed at a near sooting condition which is developed by nitrogen dilution of the flame (12).

All hydrocarbon fuel, except methane, tend to form so much soot in the standard co-flow laminar flame geometry employed that a near sooting flame is usually unattainable; with large dilution, most flames lift-off before soot formation can be eliminated. However, by simply interchanging the fuel and

oxidizer streams and choosing the dilution of the streams appropriately, stable flames with no visible soot loading are readily attained. Measurements of temperature and intermediate hydrocarbon species for these so-called "inverse diffusion flames" (IDFs) of ethene, propene and 1-butene in near and slightly sooting conditions have been made. The effects of flame temperature and fuel structure on these profiles have also been measured.

The ready achievement of an inverse diffusion flame measurement makes a description of the experimental apparatus worthwhile in this part of the research. The geometry of the burner is similar to that of previous investigations (22) on "normal diffusion flames" (NDFs) and consists of a 1 cm diameter stainless steel central tube and an 8 cm outer shroud. The oxidizer is a controllable mixture of O_2 and N_2 and flows through the central tube. The fuel flows in the outer stream and is heavily diluted with N_2. The inlet velocities of the two streams are always comparable.

The system is enclosed by a plexiglass chimney with mounted sampling probes and thermocouples fixed with respect to the chimney. The system is sealed to prevent ambient air contamination of the fuel. The entire chimney assembly is movable vertically and the probes are mounted on vernier scales so that profiles both axially (by moving the chimney) and radially are possible.

Gaseous samples were taken using an uncooled quartz micro-probe with an orifice of roughly 75 micrometers. The probe is vertical in the flame environment, roughly parallel to the streamlines. Samples are expanded from the flame to approximately 100 torr and subsequently compressed to 1 atmosphere for analysis using an HP-5840 Gas Chromatograph employing an FID. The GC/MS system was used to identify some unknown species. Some measurements of the permanent gases O_2, N_2, CO and CO_2 were made with a Varian 920 GC

employing a TCD. H₂ concentrations were not measured.

Temperature measurements were made with a 6% Rh-Pt/30% Rh-Pt thermocouple with a 0.002 inch wire and coated with quartz to a diameter of 0.004 inches to prevent catalytic effects. No corrections for conduction or radiation were made.

Of all the fuels tested, one ethene flame was sampled in detail and is considered as a base flame from which the effects of perturbations of the flame conditions can be observed. In all cases, the flame structure is kept similar by keeping the flame height and the parameter $S=X_{o_2}/[X_f(n+m/4)]$ constant. X_{o_2} and X_f are the oxygen and fuel inlet mole fractions, and n and m are the carbon and hydrogen number of the fuel (16). For a given fuel, by changing the O₂ and fuel concentrations together, flames of similar structure but uniformly higher temperatures are obtained so that the effects of increased temperature on intermediate hydrocarbon concentrations at fixed residence times (17) are observed.

Many of the original measurements were described in the previous annual report (18). Since most of this work is nearly completed and will soon appear as a Ph.D. Thesis (19), it appears appropriate to discuss the inverse diffusion flame results with respect to the early work on normal diffusion flames because in this manner the application of this research approach is most readily seen.

Detailed results of tests performed with normal diffusion flames (NDF) have been reported extensively in the papers listed in the references. Earlier results on the inverse diffusion flames were reported in the last annual report and a recent Ph.D. Thesis (19) as mentioned. It should be noted, since the objectives of the two efforts were different, that the same

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and indicates that the chemis ry depicted for C₄ species by Frenklach, et al. (20) is a common feature. At first glance it might be thought that di-acetylene is the important precursor specie for soot since its concentration is the same for all flames just prior to soot inception. However, it must be emphasized that the initial number density of soot particles formed is responsible for the soot formation rates observed in flames. If a specific specie controlled whether or not inception occurred, and that specie had similar concentrations in different flames (such as di-acetylene), the subsequent soot formation rates should be the same also. Based on this argument, di-acetylene is clearly not a controlling specie since the soot formation rates in the flames are drastically different.

The explanation for di-acetylene being similar in all flames is that di-acetylene is closely tied to both acetylene concentrations and local temperature. In an ethene JDF test with argon to separate fuel concentration from temperature effects, it was observed that di-acetylene concentrations, unlike most other species, were closely tied to temperature, and little affected by fuel concentration. Also, the ratio of di-acetylene to acetylene was observed to be very similar in all flames (implying that acetylene also has similar concentrations, which is to a large extent true). Modelling results (Singh and Kern (21) and Frenklach et al. (20) demonstrate that, as observed in these flames, an equilibrium between acetylene and di-acetylene tends to be approached.

While the inception of soot is tied to the location of the '1300K' isotherm, except for methane, the soot formation rates are related to the concentration field at inception. In particular, the aromatic content of the flames seems to scale with soot loading. In order to observe this result more

closely, Figure 3 is a plot of the fuel's sooting tendency as a function of the measured aromatic concentrations prior to soot inception. The sooting tendency is obtained from previous smoke height tests at a common inverse flame temperature of 4.32 (2315K). The results of both IDF and NDF tests indirectly confirm that the initial number density of soot particles which form scale with the aromatic content just prior to soot inception. It is not surprising that the aromatic content is so important to the soot loading. What is unique is that the aromatic content does not determine whether or not inception will occur (provided a threshold of intermediates specie concentrations exists). The results of the smoke height tests using mixtures of benzene and hexene (22) are in agreement with these observations. Adding small amounts of benzene to hexene probably does not change the location of the soot inception point, but increases the number density of particles formed there and therefore increases the sooting tendency proportionally.

Again more extensive details will be reported in the Ph.D. thesis of Sidebotham (19) and papers to be submitted. In the thesis preliminary work on the effect of small concentrations of oxygen on the sooting tendency of fuels and the possible effect of this oxygen on the chemical route to the important aromatic precursor was initiated. Such work will form one aspect of the continuing effort to gain further insight to the soot precursor formation mechanism in real flames. Other matters to be considered are the effect of diluents, hydrogen addition and possible synergistic effects of fuel mixtures. These efforts will not only give insight to the soot formation in laminar flames, but will be appropriate to understanding soot phenomena under turbulent flame conditions.

C. High Energy Density (Boron) Slurry Vaporization/Combustion Processes

    1. Free Slurry Droplet Combustion

The experimental studies in burning of free slurry droplets have progressed substantially during the past year.

Despite the considerable attention that boron slurries have received in recent years as potential high energy density liquid fuels, very little fundamental work on the actual vaporization/combustion of isolated droplets have been reported to date. The primary purpose of the current study is to investigate the fundamental vaporization/combustion behavior of boron slurry droplets and to provide information useful for fuel and combustor development efforts. First observations on the combustion properties of isolated boron slurry droplets were reported in the previous contract period [23-25], particularly focused on disruption phenomena of the primary slurry droplets. During the past year, the work was extended to in-house boron/JP-10 slurries with and without surfactants. The results were reported at the Boron Combustion Workshop at the 1987 AFOSR/ONR Contractors Meeting on Combustion [26]. Currently, some additional experimental efforts are under way to test several in-house boron/JP-10 slurries using various types of boron particles and their dispersants and to collect condensed-phase combustion products to investigate both the role of condensation and the mechanism of disruption.

Observations of burning free droplets of both pure JP-10 and boron/JP-10 slurry fuels were made in a high-temperature, atmospheric-pressure, oxidizing environment under conditions of low Reynolds number. A stream of well-dispersed droplets (approximately 100 droplet diameters apart) was projected downward through the center of a premixed, water-cooled, flat-flame burner coaxially into a hot post-combustion gas stream. A droplet generation system

utilizing an aerodynamic technique, which was developed in the previous contract period particularly for highly-viscous solid-containing liquid fuels, was used to produce small droplets (typically 350-450 microns diameter) of boron/JP-10 slurry fuels. The flat-flame burner producing the post-combustion gases was operated at atmospheric pressure using fuel-lean mixtures of methane, oxygen, and nitrogen (Table 1).

Two types of in-house boron slurries, one with a surfactant and another one without surfactant, were used in addition to a commercially available product (SunTech). Amorphous boron particles (H.C. Starck, 95/97% purity, 0.20-0.32 average diameter) were mixed with pure JP-10 (exo-tetrahydrodicyclopentadiene). A small amount (2 wt.%) of a sorbitan fatty acid ester-type surfactant (ICI Americas, SPAN85, sorbitan trioleate) was used to stabilize the slurries of the boron mass fractions of Y_B = 0.1 and 0.3.

Figure 4 shows a scanning electron micrograph (SEM) of a quasi-spherical shell of the boron agglomerate, collected from the slurry (SunTech, Y_B = 0.3) burning chimney. The diameter of the shell appears to be close to the droplet diameter at the time of disruption. The blowholes seem to be created as a result of the eruption of the mass interior of the primary slurry droplet at the disruption event. It is noticeable that the surface is relatively smooth on the outer surface of the shell as compared with the inner surface. The thickness of the shell is approximately 5-15 microns for both cases of Y_B = 0.1 and 0.3, which is slightly thinner than the estimated value (20 microns) as postulated [25]. The SEM analyses of the collected shell structure strongly support the hypotheses on the mechanisms of the formation of the impermeable shell and subsequent droplet disruption, that we have proposed previously [25](see Fig. 5).

Figure 6 shows time-exposure (1/30 s) direct photographs of disruptively-burning droplets of the in-house boron slurry with the surfactant (Y_B = 0.3, Y_{JP-10} = 0.68, Y_{SPAN85} = 0.02). Figure 3a shows the entire view of the burning process and Fig. 6b shows the magnified view of the disrupting region. The violent disruption with the greenish emission and popping sound, both which are indicative of boron ignition, was observed to be identical to the behavior of the manufactured slurries (SunTech, UOP, and Atlantic Research) as reported previously [23-25].

By contrast, as shown in Figure 7, for the slurry containing the same amount of boron (Y_B = 0.3) but no surfactant, only a weak disruption was observed at a substantially delayed time. No greenish emissions or popping sounds were noticeable and indicatesno boron ignition. The magnified view of the disrupting region (Fig. 7b) shows brushlike yellow streaks and, probably, results from puffing of gases from the primary slurry droplets. The droplets of JP-10 with 2 wt.% surfactant, tested for comparison, showed no violent disruption and the combustion terminated with the flash extinction, which was slightly stronger than pure fuels.

Figure 5 shows optical microscopic photographs of boron agglomerates collected at the exit of the combustion chimney where droplets of the in-house boron/JP-10 slurry with the surfactant are burning under the same experimental condition with that of Fig. 6. The low magnification photograph (Fig. 8a) shows the agglomerate shells with blowholes, similar to the one shown in Fig. 4, and fragments of the shells created by violent disruption. The magnified photograph (Fig. 8b) shows more clearly the shell structure and the blowholes. By contrast, as shown in Fig. 9, the structure of the agglomerates is quite different for the slurry with no surfactant collected under the same

conditions as that of Fig. 7. The agglomerates are nearly spherical and solid.

These results clearly demonstrated that the surfactant, in combination with the boron particles, is responsible for the formation of the impermeable shell structure and subsequent disruption phenomena. The physical ideas that have been proposed previously [23-25] and the observations reported here should be used to develop quantitative models for the disruptive burning process.

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TABLE 1 Burner Operating Conditions and Estimated
Gas Mixture Compositions

| X_{H2O} | Gas mix. no. | ϕ | Flow Rate (l/min) | | | $T_{f,CH4}$ (K) | X_{O2} | Mole Fraction | |
			CH_4	O_2	N_2			X_{H2}	X_{CO2}
0.17	1	0.3	10.0	66.7	43.3	2054	0.39	0.36	0.08
0.17	2	0.4	10.0	50.0	60.0	2065	0.25	0.50	0.08
0.17	3	0.5	10.0	40.0	70.0	2073	0.17	0.58	0.08
0.17	4	0.6	10.0	33.3	76.7	2078	0.11	0.64	0.08
0.17	5	0.7	10.0	28.6	81.4	2086	0.07	0.68	0.08

FIGURE CAPTIONS

Fig. 1.   Major species profiles from the oxidation of p-xylene.

Fig. 2.   Intermediates in near sooting and smoke point conditions of normal
           and inverse diffusion flames.

Fig. 3.   Fuel's sooting tendency correlated with measured aromatic
           concentration.

Fig. 4   Scanning electron micrograph of a boron agglomerate shell (100X).

Fig. 5.   Schematic illustration of the disruption mechanism.

Fig. 6.   Time-exposure photographs of burning boron/JP-10 slurry droplets
           with the surfactant. $Y_s = 0.30$, $Y_{SPANes} = 0.02$. (a) Entire view.
           (b) Magnified view.

Fig. 7.   Time-exposure photographs of burning boron/JP-10 slurry droplets
           with no surfactant. $Y_s = 0.3$. (a) Entire view. (b) Magnified view.

Fig. 8.   Photographs of boron agglomerates collected in the combustion of
           boron/JP-10 slurry droplets with the surfactant. $Y_s = 0.30$, Y_{SPANes}
           $= 0.02$. (a) Low magnification; (b) high magnification.

Fig. 9.   Photographs of boron agglomerates collected in the combustion of
           boron/JP-10 slurry droplets with no surfactant. $Y_s = 0.30$. (a) Low
           magnification; (b) high magnification.

p-Xylene Oxidation
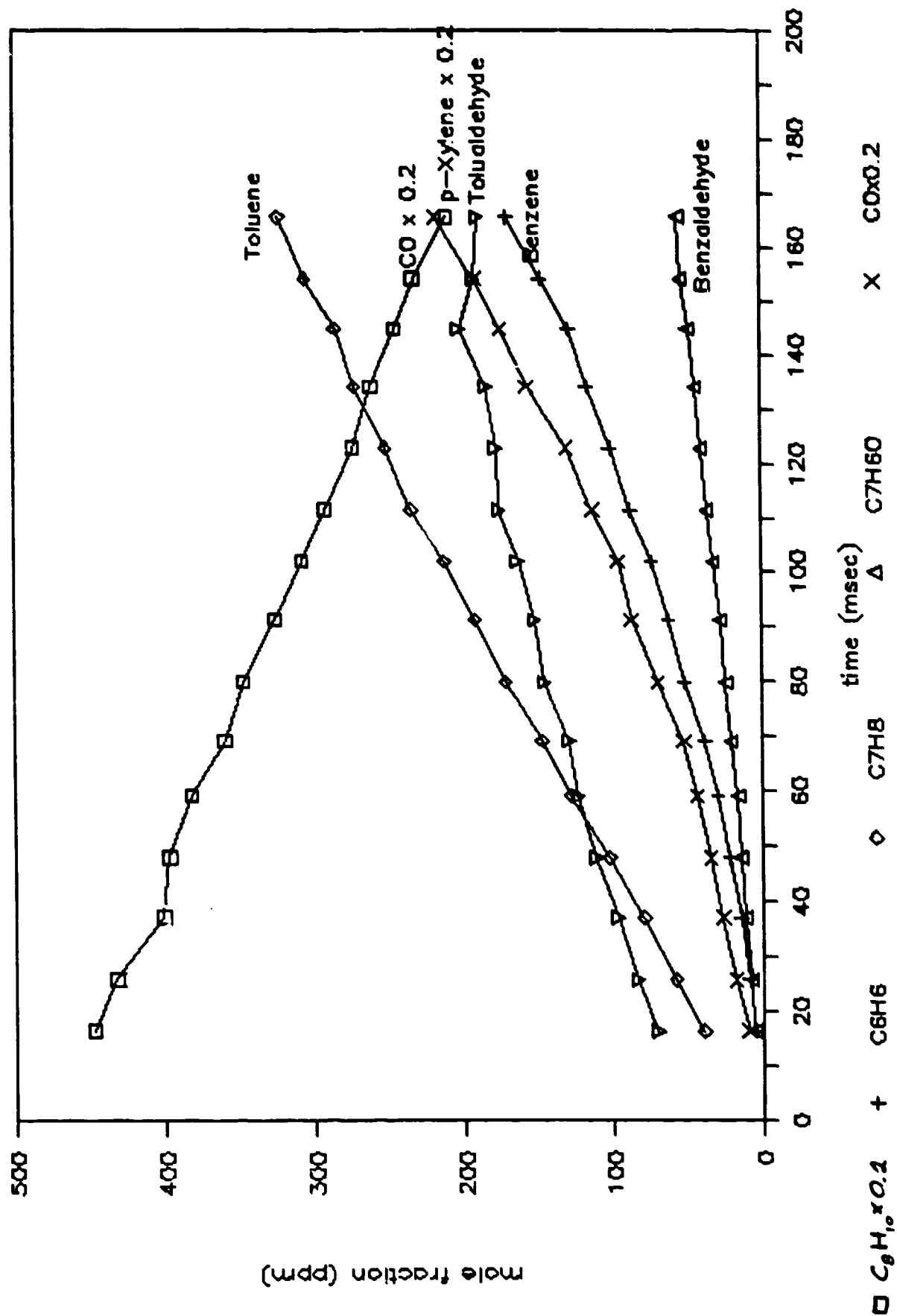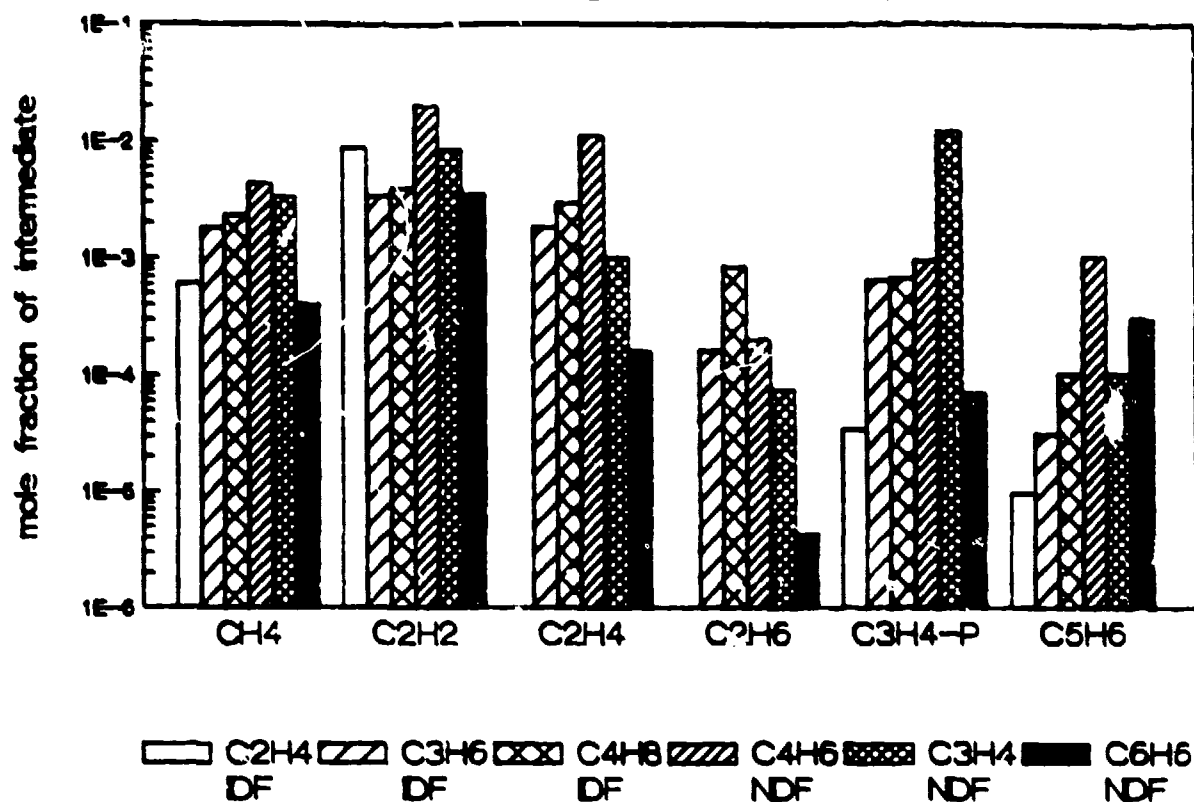### Phi=1.33 To=1163 K

Toluene

CO x 0.2

p-Xylene x 0.2
Toluadehyde

Benzene

Benzaldehyde

mole fraction (ppm)

time (msec)

$\nabla\ C_8H_{10} \times 0.2$ $+$ C6H6 $\diamond$ C7H8 $\triangle$ C7H6O $\times$ COx0.2 $\square$ $\nabla\ C_8H_2O$

Figure 1
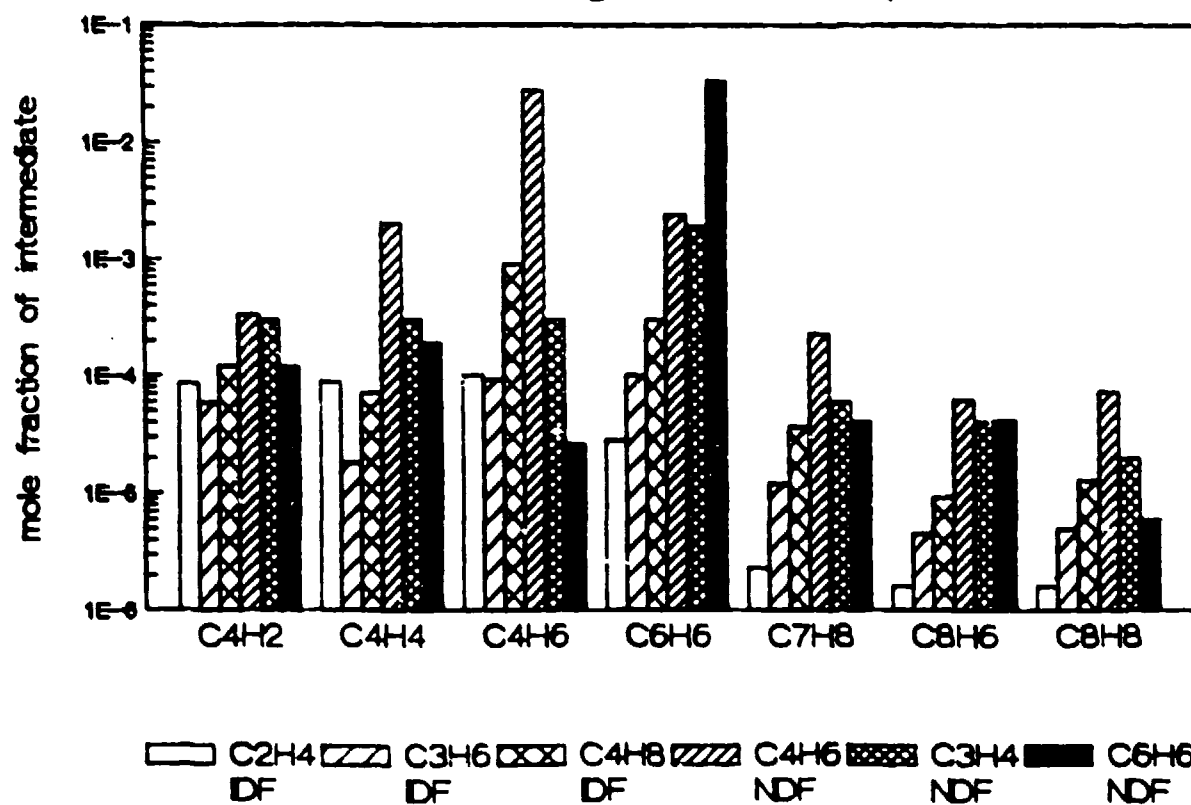
IDFs and NDFs
near sooting and smoke point

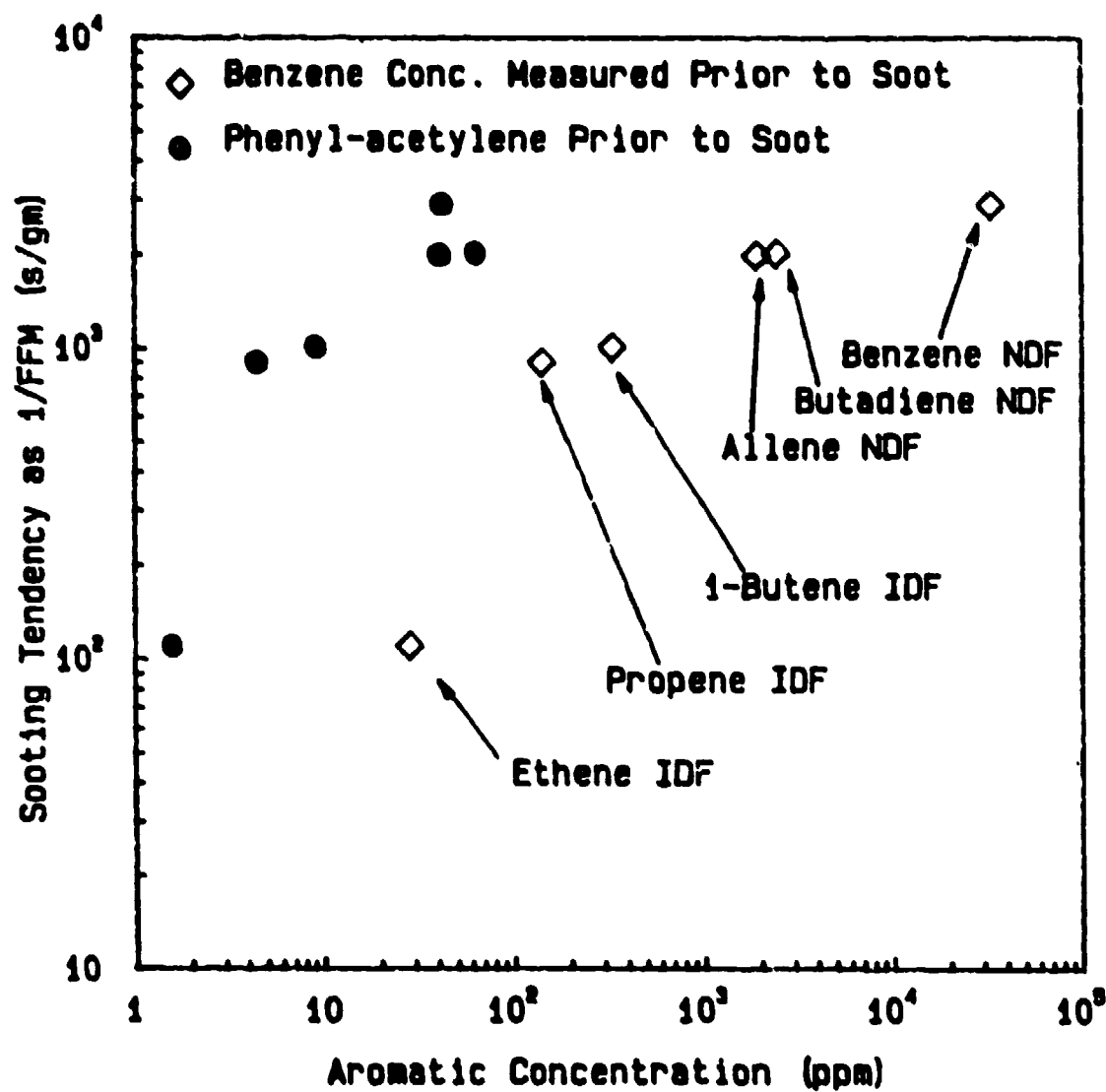# IDFs and NDFs
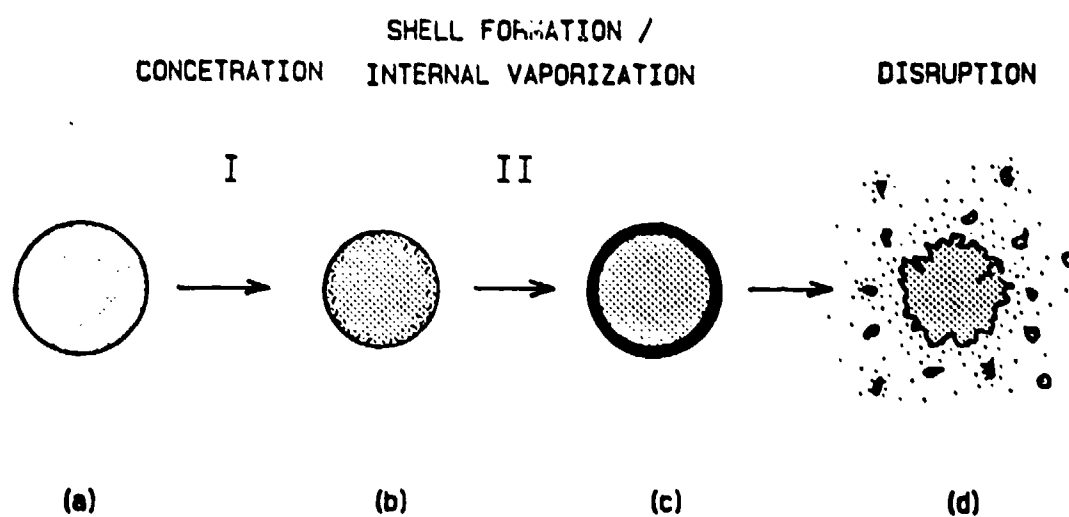## near sooting and smoke point

Figure 2

Figure 3

Figure 4

SHELL FORMATION /
CONCETRATION   INTERNAL VAPORIZATION   DISRUPTION

I   II

(a)   (b)   (c)   (d)

Figure 5

(a)

30 cm

(b)

10 cm

Figure 6

(a)
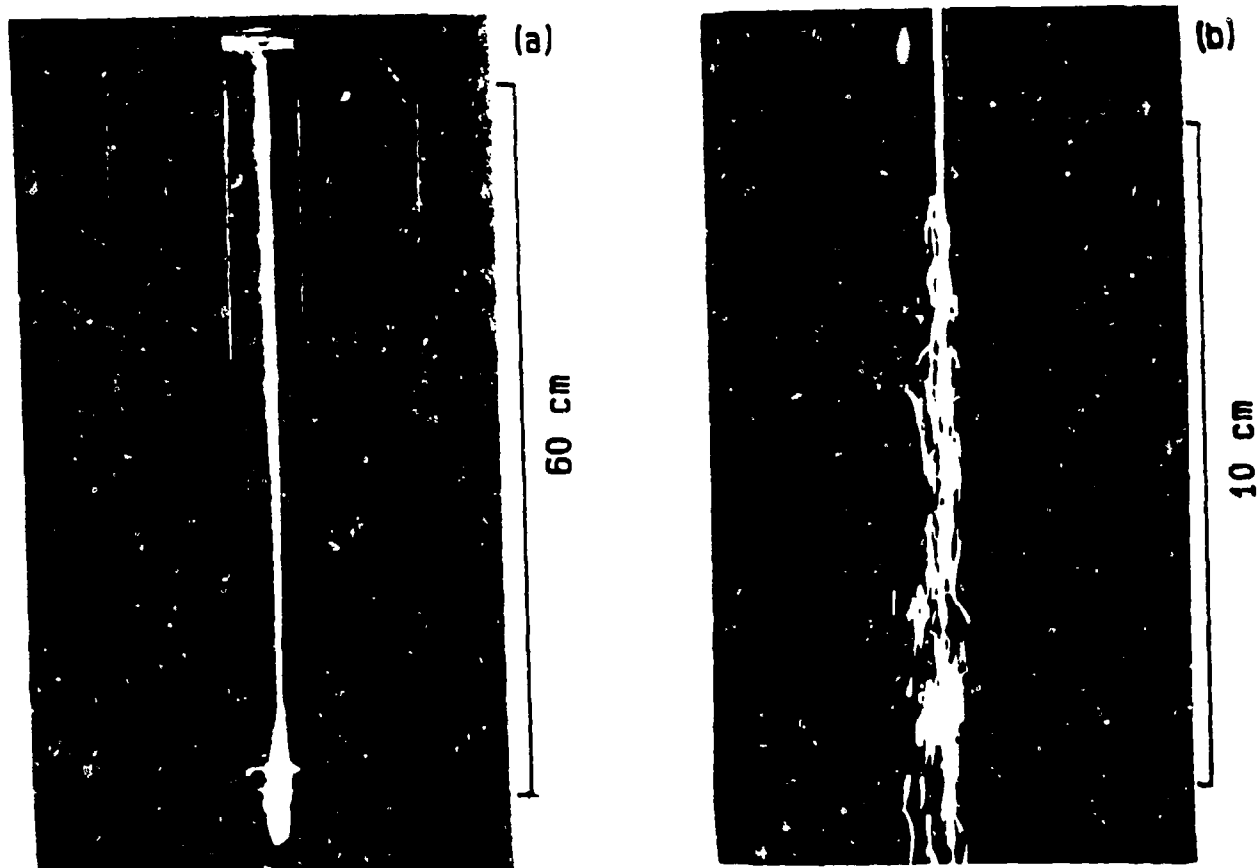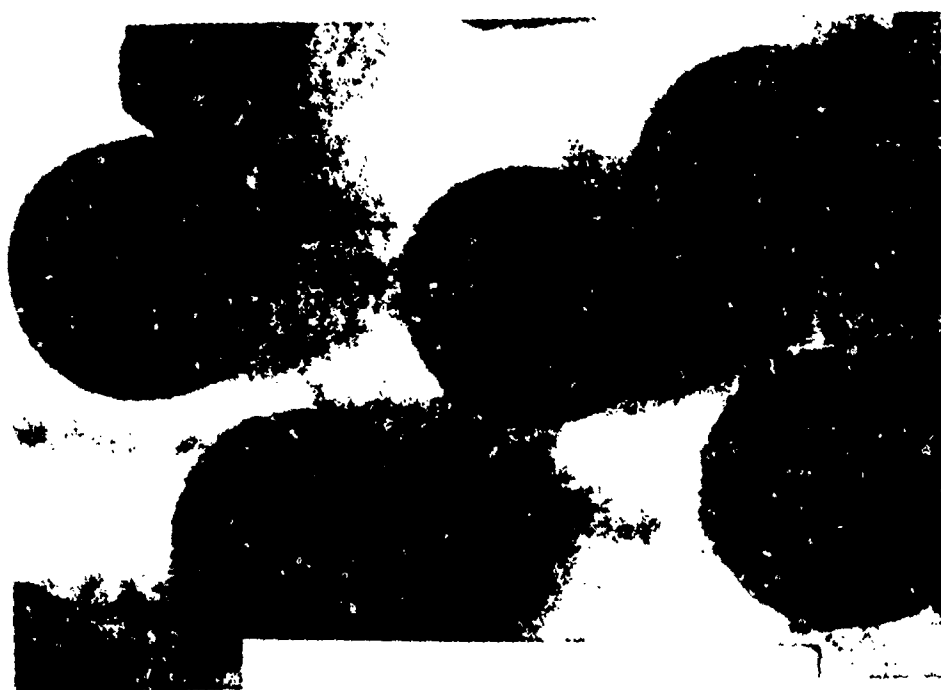
60 cm

(b)

10 cm
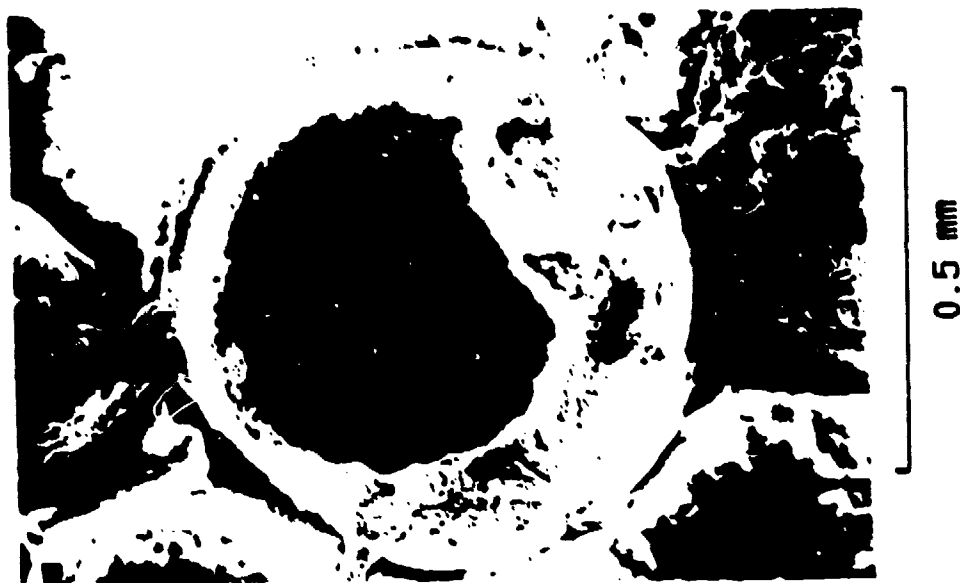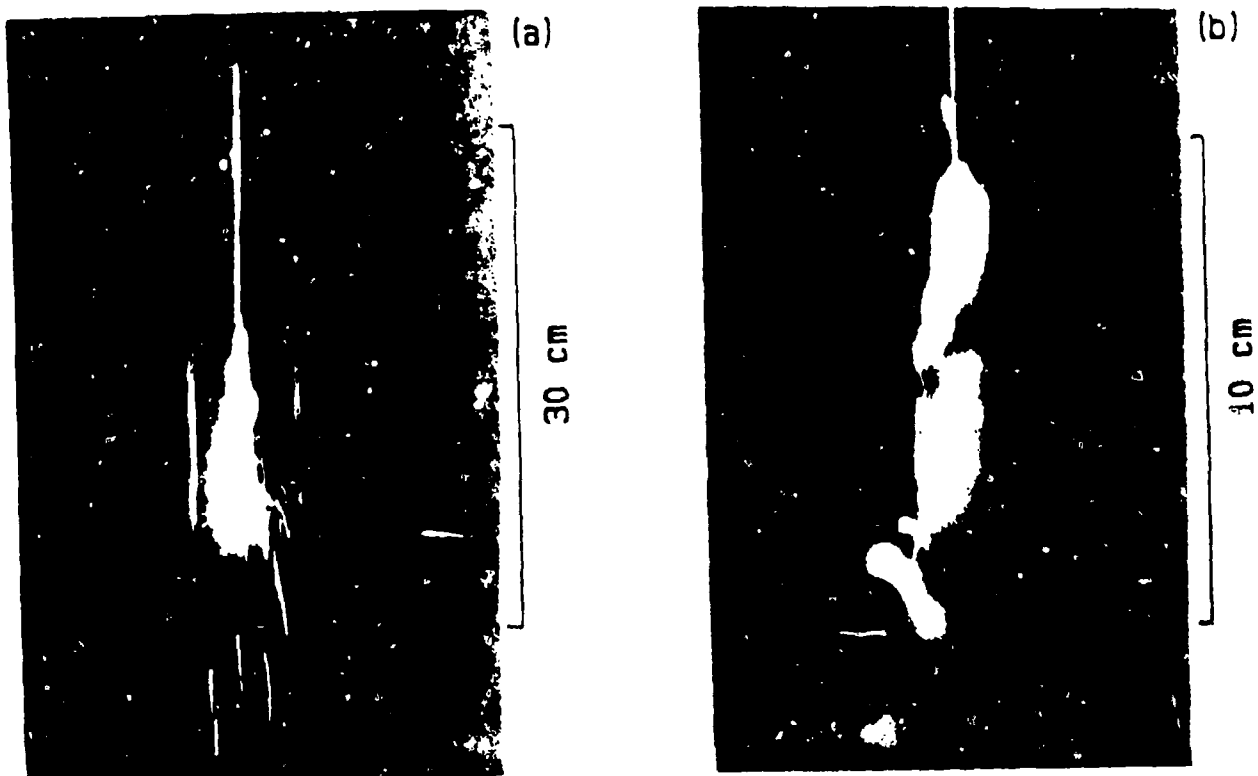
Figure 7

(a)

(b)

Figure 8

(a)

(b)

Figure 9

III. Publications Related to Current Effort

1. F... Dryer and I. Glassman, "Combustion Chemistry of Chain Hydrocarbons," in "Alternative Hydrocarbon Fuels: Combustion and Chemical Kinetics," AIAA Series of Progress in Astronautics and Aeronautics, Vol. 62, p. 255 (1978), AIAA, New York.

2. R.J. Santoro and I. Glassman, "A Review of Oxidation of Aromatic Compounds," Combustion Science and Technology 19, 161 (1979).

3. D.J. Hautman, F.L. Dryer, K.P. Schug and I. Glassman, "A Multiple-Step Overall Kinetic Mechanism for the Oxidation of Hydrocarbons," Combustion Science and Technology 25, 219 (1981).

4. C. Venkat, K. Brezinsky, and I. Glassman, "High Temperature Oxidation of Aromatic Hydrocarbons," 19th Symp. (Int'l.) on Combustion, The Combustion Institute, Pittsburgh, p. 143, (1982).

5. K. Brezinsky, T.A. Litzinger, and I. Glassman, "The High Temperature Oxidation of the Methyl Side Chem of Toluene," Int. J. Chem. Kinetics 16, 1053 (1984).

6. T.A. Litzinger, K. Brezinsky, and I. Glassman, "Some Further Results on the Toluene Oxidation Mechanism," Eastern States Section: The Combustion Institute Meeting, Paper No. 69, December 1982.

7. T.A. Litzinger, K. Brezinsky, and I. Glassman, "Some Further Results on the Oxidation of Ethyl Benzene," Eastern States Section: The Combustion Institute Meeting, Paper No. 3, November 1983.

8. T.A. Litzinger, K. Brezinsky, and I. Glassman, "A Comparison of Results from the Oxidation of Normal and Isopropyl Benzene," Eastern States Section: The Combustion Institute Meeting, Paper No. 90, November 1984.

9. T.A. Litzinger, K. Brezinsky and I. Glassman, "The Role of Selectivity for Radical Abstraction of Hydrogen Atoms in the Oxidation of Normal and Isopropyl Benzene", to be presented at the International Conference on Chemical Kinetics, National Bureau of Standards, June 1985.

10. A. Gomez, G. Sidebotham and I. Glassman, "Sooting Behavior in Temperature Controlled Laminar Diffusion Flames," Comb. and Flame 58, 45 (1984).

11. K. Brezinsky, E.J. Burke and I. Glassman, "The High Temperature Oxidation of Butadiene," 20th Int'l. Symposium on Combustion, p. 613 (1984).

12. I. Glassman, "Phenomenological Models of Soot Processes in Combustion Systems," AFOSR Technical Report No. 79-1147 (1979).

13. K.P. Schug, Y. Manheimer-Timnat, P. Yaccarino and I. Glassman, "Sooting Behavior of Gaseous Hydrocarbon Diffusion Flames and the Influence of Hydrocarbons, "Combustion Science and Technology 22, 235 (1980).

14. I. Glassman and P. Yaccarino, "The Effect of Oxygen Concentration on Sooting Diffusion Flames," Combustion Science and Technology 24, 107 (1980).

15. I. Glassman and P. Yaccarino, "The Temperature Effect in Sooting Diffusion Flames," 18th Int'l. Symposium on Combustion, The Combustion Institute, Pittsburgh, PA (1981).

16. Lt. K.E. van Teuren, "Sooting Characteristics of Liquid Pool Diffusion Flames," M.S.E. Thesis, Department of Mechanical and Aerospace Engineering, Princeton University (1978).

17. G. Sidebotham and I. Glassman, "Sooting Behavior of Cyclic Hydrocarbons in Laminar Diffusion Flames," Eastern States Section, The Combustion Institute Meeting, Paper No. 61, November 1983.

18. K.P. Schug, Y. Manheimer-Timnat, P. Yaccarino and I. Glassman, "Sooting Behavior of Gaseous Hydrocarbon Diffusion Flame and the Influence of Hydrocarbons," Combustion Science and Technology 22, 235 (1980).

19. I. Glassman and P. Yaccarino, "The Temperature Effect in Sooting Diffusion Flames," 18th Int'l. Symposium on Combustion, The Combustion Institute, Pittsburgh, PA (1981).

20. G. Sidebotham and I. Glassman, "Soot Formation in Laminar Diffusion Flames of Benzene II-Hexene Mixtures," Eastern States Section: The Combustion Institute Meeting, Paper No. 97, December 1985.

21. F. Takahashi and I. Glassman, "Sooting Correlations for Premixed Flames," Eastern States Section: The Combustion Institute Meeting, Paper No. 56, December 1982.

22. F. Takahashi and I. Glassman, "Interpretation of Sooting Correlations Under Premixed Conditions," Eastern States Section: The Combustion Institute Meeting, Paper No. 12, November 1983.

23. F. Takahashi and I. Glassman, "Sooting Correlations for Premixed Flames," Combustion Science and Technology 37, 1 (1984).

24. F. Takahashi, J. Bonini, and I. Glassman, "Further Experiments and Analysis of the Sooting Tendency of Premixed Fuels," Eastern States Section: The Combustion Institute Meeting, Paper No. 98, December 1985.

25. I. Glassman, F.A. Williams and P. Antaki, "A Physical and Chemical Interpretation of Boron Particle Combustion," 20th Int'l. Combustion Symposium, p. 2057 (1984).

26. P. Antaki, "Transient Processes in Slurry Droplets During Liquid Vaporization and Combustion," Eastern States Section, The Combustion Institute Meeting, Paper No. 62, December 1984.

27. P. Antaki, "Transient Processes in a Rigid Slurry Droplet During Liquid Vaporization and Combustion," Combustion Science and Technology, 46, 113 (1986).

28. F. Takahashi, F.L. Dryer and F.A. Williams, "Combustion Behavior of Free Boron Slurry Droplets," Central and Western States Section, The Combustion Institute Meeting, Paper No. 2-2B, April 1985.

29. Y.T. Loo, I.M. Kennedy and F.L. Dryer, "Disruptive and Micro-explosive Combustion of Free Droplets in Highly Connective Environments," Combust. Sci. and Tech. 41, 291 (1984).

30. P. Antaki, "Transient Processes in a Non-Rigid Slurry Droplet During Liquid Vaporization and Combustion," Combust. Sci. and Tech. 49, 289 (1986).

31. A. Gomez, M. Littman and I. Glassman, "Comparative Study of the Sooting Behavior of an Aromatic Versus an Aliphatic in Diffusion Flames," Western States Section/The Combustion Institute, Paper No. 6-7A (1986).

32. T.A. Litzinger, K. Brezinsky and I. Glassman, "Reaction of n-Propyl Benzene During Gas Phase Oxidation," Comb. Sci. and Tech. 50, 117 (1984).

33. T.A. Litzinger, K. Brezinsky and I. Glassman, "Gas Phase Oxidation of Isopropylbenzene at High Temperature," J. of Phys. Chem. 90, 508 (1986).

34. T.A. Litzinger, K. Brezinsky and I. Glassman, "Preliminary Experiments with 1-Methylnaphthaline near 1180K," Eastern States Meeting/The Combustion Institute Paper No. 68 (1985).

35. I. Glassman, "Physical and Chemical Effect in Soot Formation," Eastern States Meeting/The Combustion Institute Invited Paper D (1985).

36. K. Brezinsky, G.F. Linteris, T.A. Litzinger and I. Glassman, "High Temperature Oxidation of n-Alkyl Benzene," accepted for publication in 21st Symp. (Int'l.) on Combustion.

37. G.W. Sidebotham and I. Glassman, "Structure of Near and Slightly Sooting Inverse Diffusion Flames," accepted for presentation at 1986 Eastern States/The Combustion Institute Meeting, Paper No. 34 (1986).

38. F. Takahashi, F.L. Dryer and F.A. Williams, "Combustion Behavior of Free Boron Slurry Droplets," AFOSR TR-85-0559, May 1985.

39. F. Takahashi, F.L. Dryer and F.A. Williams, "Further Experiments on the Combustion Behavior of Free Boron Slurry Droplets," Eastern States Section: The Combustion Institute Meeting, Paper No. 19, November 1985.

40. F. Takahashi, F.L. Dryer and F.A. Williams, Combustion Behavior of Free Boron Slurry Droplets," Twenty-First Symposium (Int'l.) on Combustion, The Combustion Institute, Pittsburgh, PA, 1986 (in press).

41. K. Brezinsky, "The High Temperature Oxidation of Aromatic Hydrocarbons," Prog. in Energy and Combust. Sci. 21, 1 (1986).

42. P. Antaki and F.A. Williams, "Transient Processes in a Non-Rigid Slurry Droplet During Liquid Vaporization and Combustion," Combustion Science and Technology, 49, 289 (1986).

43. P. Antaki and F.A. Williams, "Observations on the Combustion of Boron Slurry Droplets in Air," Combustion and Flame, to appear (1986).

44. G.W. Sidebotham, K. Saito, I. Glassman, and A.S. Gordon, "An Experimental Study of Allene, 1-3 Butadiene and Benzene Laminar Co-Flowing Diffusion Flames," Central States Section/Combustion Institute Meeting, Spring 1987.

45. K. Brezinsky and I. Glassman, "Oxidation/Pyrolysis Chemistry as Related to Fuel Sooting Tendencies," to appear in Energy and Fuel.

IV. Professional Personnel and Graduate Students Theses

Prof. F.L. Dryer
Prof. I. Glassman, Coordinator
Prof. F.A. Williams
Dr. K. Brezinsky
Dr. F. Takahashi

1. D.J. Hautman, "Pyrolysis and Oxidation Kinetic Mechanisms for Propane," Department of Mechanical and Aerospace Engineering, Ph.D. Thesis (1980).

2. J.A. Euchner, "A Study of the Oxidation of Toluene in a Flow Reactor," Department of Mechanical and Aerospace Engineering, M.S.E. Thesis (1980)

3. S.L. Murphy, "Pure and Oxidative Pyrolysis of Hydrocarbons in Relation to the Sooting Diffusion Flame," M.S.E. Thesis, Department of Mechanical and Aerospace Engineering, August 1982.

4. E.J. Burke, "A Study of the High Temperature Oxidation of 1,3-Butadiene," M.S.E. Thesis, Department of Mechanical and Aerospace Engineering, Princeton University, 1983.

5. P. Yaccarino, "Parametric Study of Sooting Diffusion Flames," Department of Mechanical and Aerospace Engineering, M.S.E. Thesis (1980).

6. Lt. K.E. van Teuren, "Sooting Characteristics of Liquid Pool Diffusion Flames," M.S.E. Thesis, Department of Mechanical and Aerospace Engineering, Princeton University (1978).

7. C. Venkat, "High Temperature Oxidation of Aromatic Hydrocarbons," Department of Chemical Engineering, M.S.E. Thesis (1981).

8. T. Litzinger, "The High Temperature Oxidation of Alkylated Aromatic Hydrocarbons," Department of Mechanical and Aerospace Engineering, Ph.D. Thesis (1985).

9. P. Antaki, "Studies of Slurry Droplet Combustion and Boron Particle Ignition," Department of Mechanical and Aerospace Engineering, Ph.D. Thesis (1985).

10. G.W. Sidebotham, "An Inverse Co-Flow Approach to Sooting Laminar Diffusion Flames," Department of Mechanical and Aerospace Engineering, Ph.D. Thesis (1987).

V. Presentation - Seminars

K. Brezinsky

"Chemical Species Measurements in a High Temperature Flow Reactor," Standard Oil Research and Development, Warrenville, OH, March 19, 1987.

"Oxidation and Pyrolysis Chemistry of Hydrocarbon Fuels," GM Research Laboratories, Warren, MI, June 18, 1987.

"Oxidation/Pyrolysis Chemistry as Related to Fuel Sooting Turbulences," American Chemical Society, National Meeting, Sept. 1, 1987, New Orleans, LA.

G. Sidebotham

"Structure of Near and Slightly Sooting Inverse Diffusion Flames; Eastern States Section/Combustion Institute Meeting, Dec. 16, 1986, San Juan, P.R.

"An Experimental Study of Allene, 1-3 Butadiene and Benzene Laminar Co-Flowing Diffusion Flames," Central States Section Combustion Institute Meeting, May 12, 1987, Argonne, IL.

F. Takahashi

"Combustion Behavior of Free Boron Slurry Droplets," Boron Workshop, 1987 AFOSR/ONR Contractors Meeting, June 23, 1987, University Park, PA.

VI. Interaction With Other Laboratories

Discussion about soot formation in dump combustors with NASA Langley, June 1987.

Discussion about soot formation in aircraft gas turbines with AVCO-Lycoming, UTRC, McDonnell-Douglas, June 1987.

Discussions about hydrocarbon oxidation processes with Standard Oil Research and G.M. Research, March-June 1987.